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Quadrupolar Order in the Quantum XY Model with Cubic Anisotropy

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We present a new algorithm for the quantum $S = 1$ XY model with cubic anisotropy. In two dimensions, by studying the behaviour of the quadrupolar moment, we find the magnitude of the anisotropy at which a presumably ferromagnetic phase terminates. This point coincides with the phase boundary between the ferromagnetic phase and the quadrupolar phase determined by the mean-field theory. However, in contrast to the mean-field prediction, there is no quadrupolar phase just above the phase boundary.

§1. Introduction

The nature of real magnetic materials are affected by the various types of anisotropy. A number of works have been done on the effects of anisotropy. The anisotropy effect in the quantum case can be qualitatively different from that in the classical case. For example, recently, M. Dudzinski and J. Sznajd predicted that if the anisotropy is sufficiently strong there is a non-magnetic ordered phase with spontaneous quadrupolar order even at zero temperature.¹⁾ This is interesting because their model Hamiltonian has no term which explicitly enhances the quadrupole-quadrupole correlation, and accordingly the quadrupolar phase does not exist in the classical case at zero temperature. In other words, they suggested that the coexistence of the anisotropy and the quantum effect may cause a new zero-temperature phase.

While there are some theoretical studies as mentioned above, the direct numerical studies are missing in particular for quantum spin models. The anisotropic term in the Hamiltonian is represented by the higher-order term of spin operators. It was difficult to simulate models with these complex terms by the Quantum Monte Carlo (QMC) methods. The recent progress of QMC algorithm, however, made it possible in some cases. For example, we studied²⁾ the Heisenberg models with the bi-quadratic interaction terms, although it still possesses the $SU(2)$ symmetry unlike the case we are studying in the present paper. The phase diagrams and critical exponents were numerically calculated in order to check the various theoretical predictions.

In this paper, we present a new algorithm for the quantum $S = 1$ XY model with a cubic anisotropy term, which reduces the models symmetry from $U(1)$ to tetragonal, and show some results of simulations on a square lattice. We also compare our results with the phase diagram determined by the mean-field theory.

§2. Quantum XY model with cubic anisotropy

Our model for the quantum XY model with the cubic anisotropy in two dimensions is defined by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} [S_i^x S_j^x + S_i^y S_j^y] - D \sum_{\langle ij \rangle} [(S_i^x)^2 (S_j^x)^2 + (S_i^y)^2 (S_j^y)^2 + (S_i^z)^2 (S_j^z)^2], \quad (2.1)$$

where spin operators on site i are denoted by S_i^α , and the $\langle ij \rangle$ runs over all nearest-neighbour pairs on a square lattice. In what follows, we consider the case where the coupling constants J and D are positive.

For the anisotropy term, we take the one which usually represents the cubic anisotropy. While we could drop the term $(S_i^z)^2 (S_j^z)^2$ without changing the symmetry of the whole Hamiltonian, we speculate that it would not make a qualitative difference. The anisotropy term is equivalent to a constant when the spin length S is $1/2$. In the present paper, therefore, we discuss the case $S = 1$ because our interest is in the interplay between strong quantum fluctuation and anisotropy.

It is well known that the classical non-anisotropic XY model in two dimensions has the phase transition of the Kosterlitz-Thouless type predicted by the renormalization group theory,⁴⁾ and it has been also confirmed through numerical simulation in the quantum case.⁵⁾ However, our understanding of the model with an anisotropy term is limited. For the cubic anisotropy case, we calculated the phase diagram by the mean-field approximation.³⁾ As we can see in Fig. 1, there are two phases at low temperature, whose boundary is at $D = 2J$. In the weak anisotropy region ($2J > D > 0$), there is the ferromagnetic phase in which the dipole moment is finite. In the strong anisotropy region ($D > 2J$), on the other hand, there is no finite dipole moment whereas the quadrupolar moment is finite. The phase transition from the paramagnetic phase to the quadrupolar phase is always of the first order, and it is the case also in the weak anisotropy region near the $D = 2J$ point. But as the anisotropy becomes sufficiently weak, the transition becomes second order. For this second order transition, J. V. Jose et al. predicted that the values of the critical exponents continuously change.⁶⁾

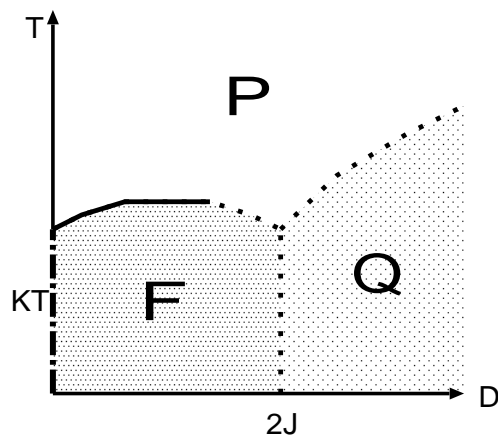


Fig. 1. The schematic phase diagram by the mean-field approximation. The symbols “P”, “F” and “Q” denote the paramagnetic, ferromagnetic and quadrupolar phase respectively. The solid (dotted) line corresponds to the first (second) order phase transition.

§3. Loop algorithm for the quantum $S = 1$ XY model with cubic anisotropy

Quantum Monte Carlo methods based on the world-line representation were formulated in the early eighties and have been successfully applied to quantum spin systems since.⁷⁾ The recent QMC algorithms, such as the loop algorithm,⁸⁾ consist of non-local updates of the spin configuration or the world-line configurations. Their relaxation times are usually much smaller than that of the conventional algorithm, and, when the continuous imaginary time scheme is adopted,⁹⁾ they have no systematic errors due to the discretization of imaginary time integral. Therefore, we can do high-precision numerical simulations for quantum spin systems at low temperature.

The loop algorithms are usually constructed for the Hamiltonian matrix represented in the basis which diagonalizes the S_i^z . It was firstly formulated only for the quantum $S = 1/2$ spin systems. But it is possible to apply it to the quantum spin systems with larger spins by decomposing the one original spin into $2S$ Pauli spins.¹⁰⁾

In general, the loop algorithm consists of two procedures: (i) placing graphs on the world-line configurations by a Poisson process whose density depends on the Hamiltonian matrix and (ii) flipping loops formed in the procedure (i) independently with the probability $1/2$. The flipping of these loops, instead of flipping single spin, often reduces the correlation times at low temperature. The number of distinct types of graph is usually very few. For example, in the case of the isotropic (i.e. $U(1)$ symmetric) XY model, we need only first two types of graphs among the three in Fig. 2.

To accommodate the cubic anisotropy term, we need the last type of graph. Graphs of this type obviously cause branching of the lines, turning loops into clusters. Therefore, it often happens that one particular cluster contains almost all the spins in the system at low temperature and the computational correlation times become very large. This makes it impossible to do high-precision numerical simulations. In order to avoid this difficulty, we use the new basis which diagonalizes the cubic anisotropic terms:

$$|+\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |-1\rangle), \quad |0\rangle, \quad |-\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |-1\rangle). \quad (3.1)$$

Although the XY model term does not have the negative sign problem in this new basis, the Heisenberg model does, which is the another reason for studying the XY model instead of the Heisenberg model. The new loop algorithm has three steps: (i)

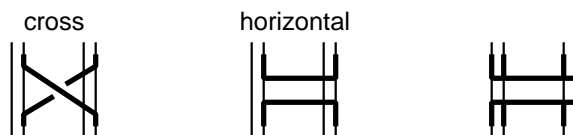


Fig. 2. Graphs in the loop algorithm on the basis which consists of eigenstates of the z -direction spin operators. The vertical direction corresponds to the imaginary time.

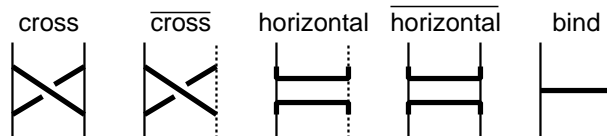


Fig. 3. Graphs in the new loop algorithm. The vertical solid and dashed lines denote the two spin states selected in the step (i).

randomly selecting two states among the three $|+\rangle$, $|0\rangle$ and $|-\rangle$ to be updated, (ii) placing graphs on top of the world-lines of their states, (iii) each loop is independently flipped. In doing so, we must fix the loop whose flipping would result in the states corresponding to vanishing matrix elements of the Hamiltonian matrix in the new basis. We use the graphs in Fig. 3 for the present model. The density of the Poisson process for placing each type of graphs is shown in Table I. As can be seen in Table I, the types of graphs are changed at $D = 2J$ which is the physical phase boundary in the mean-field predictions. The correspondence between the algorithmic and physical boundaries is also observed in other models as well.²⁾ It is related to the symmetry or anisotropy of the model.

Table I. Strength of the Poisson distribution of graphs.

Updated pair	G_{cross}	$G_{\overline{\text{cross}}}$	$G_{\text{horizontal}}$	$G_{\overline{\text{horizontal}}}$	G_{bind}
$(+, 0)$ or $(-, 0)$ when $D > 2J$	J	0	J	0	$D - 2J$
$(+, 0)$ or $(-, 0)$ when $D \leq 2J$	$J/2 + D/4$	$J/2 - D/4$	$J/2 + D/4$	$J/2 - D/4$	0
$(+, -)$	0	0	0	0	D

§4. Simulations

We have performed simulations at various magnitudes of anisotropy, D , on the square lattices with $L = 4, 8, 16, 32, 64$. Each run is of more than 10^4 Monte Carlo sweeps. In our simulations, we have measured the energy, the specific heat and the quadrupolar moment

$$Q_{xy} \equiv S_{x,i}^2 - S_{y,i}^2. \quad (4.1)$$

Unfortunately, the magnetization cannot be measured except at the $D = 2J$ point, even if we use the improved-estimator method¹¹⁾ for computing the off-diagonal Green's function.

In Fig. 4, we plot the thermodynamic averages of the absolute value of the quadrupolar moment on the square lattice for $L = 32$ at various values of $D/2J$. The behaviour of the quadrupolar moment at low temperature clearly changes at the $D = 2J$ point.

Below this value, the quadrupolar moment increases as temperature decreases until it reaches the saturated value near zero temperature (Figs. 4 and 5). This indicates some spontaneous symmetry breaking in this region. We suspect that this phase is the ferromagnetic phase because it is supposed to be so at least for very small anisotropy,⁶⁾ and there is no clear qualitative change in the temperature dependence

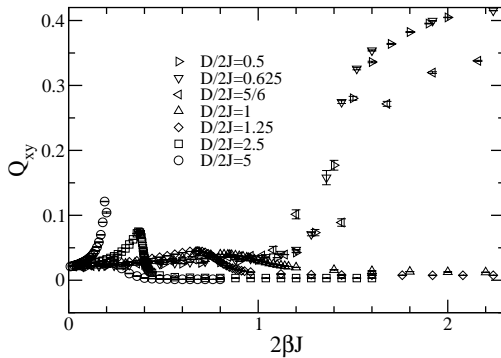


Fig. 4. Quadrupolar moment on the square lattice with $L = 32$.

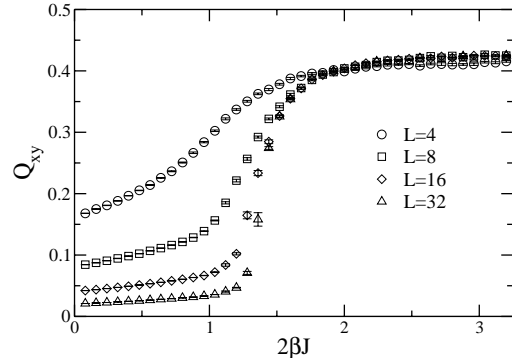


Fig. 5. Quadrupolar moment at $D/2J = 0.625 < 1$.

of the quadrupolar moment in the whole region of $0 < D < 2J$. However, we cannot really confirm that this is the case since we cannot directly measure the magnetization as stated above. The continuously changing critical exponents predicted by Jose et al. are another issue of interest here. However, the results of the present simulations are not enough for us to determine whether the phase transition in the weak anisotropy region is of the first or the second order or whether the values of the critical exponents continuously change or not. We are still continuing additional simulations and the results will be reported elsewhere.

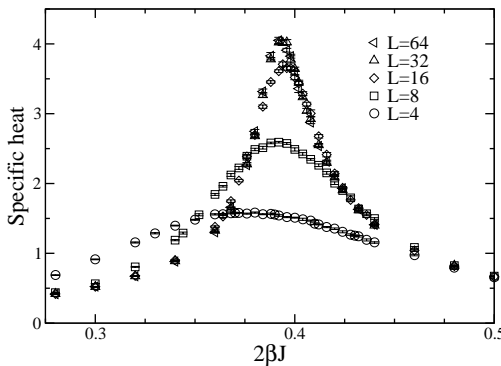


Fig. 6. Specific heat at $D/2J = 2.5 > 1$.

The value $D/2J = 1$ agrees with the mean-field phase boundary between the ferromagnetic phase and the quadrupolar phase. However, in the strong anisotropy side of this boundary, the values of the quadrupolar moments show somewhat strange behaviour which is quite unlikely for the quadrupolar phase. As the temperature is lowered it increases initially, but starts to decrease at some temperature and rapidly converges to zero at lower temperatures. We know, on the other hand, that there is the quadrupolar phase at low temperature in the limit

of strong anisotropy, since the model with $J = 0$ is equivalent to the classical 3-state Potts model, which does have a phase transition at a finite temperature.

In order to see if a phase transition exists at a finite temperature for strong but finite anisotropy, we computed the specific heat at $D/2J = 2.5 > 1$ (Fig. 6). The peak is observed near the temperature at which the quadrupolar moment at $J = 0$. The peak height and width show a significant size dependence for small systems but seem to converge as the system becomes larger. This may indicate that the sharp

peak in the specific heat is not of a phase transition but only of a crossover.

§5. Conclusion

We have presented a new loop algorithm for the quantum $S = 1$ XY model with the cubic anisotropy term, and done numerical simulations in two dimensions. In contrast to the mean-field prediction, the phase transition to the quadrupolar phase is missing at least for some finite region just above the boundary $D = 2J$, and we did not observe any evidence for its presence at any value of D although it is technically difficult in the present case to distinguish between a mere crossover and a phase transition. On the other hand, in the weak anisotropy region, there is a phase transition from the paramagnetic phase to the phase with spontaneously broken symmetry, presumably the ferromagnetic phase. We are still working on the refinement of the D/J - T phase diagram of the present model. In addition, studies of other anisotropic models are also in progress. They will be reported elsewhere.

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